Crystal Lattice Structures:

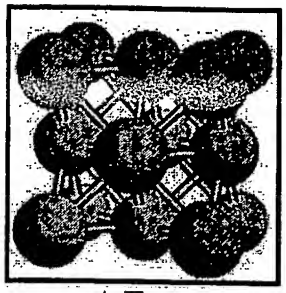
Reference Date: 1 Sep 1995
Last Modified: 21 Oct 2004

Index by *Strukturbericht* Designation

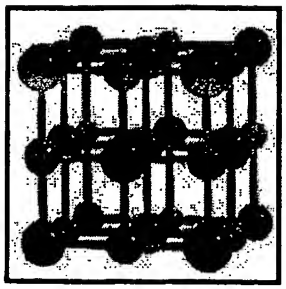
- *Strukturbericht* symbols are a partly systematic method for specifying the structure of a crystal. Thus the A structures are supposed to be monatomic, B's are diatomic with equal numbers of atoms of each type, C's have a 2-1 abundance ratio, D0's are 3-1, etc. Unfortunately, this scheme breaks down as early as A15. Numbers were assigned in roughly the historical order of the study of the lattice.
- Barrett and Massalski give a table (p. 29) which gives the correspondence between the *Strukturbericht* types and the complexity of the crystal:

***Strukturbericht* Designation**	**Crystal Type**
A	Elements
B	AB compounds
C	AB_2 compounds
D	A_mB_n compounds
E, F, G, H ··· K	More complex compounds
L	Alloys
O	Organic compounds
S	Silicates

Strukturbericht Types:



A Type



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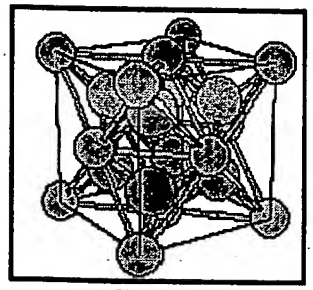
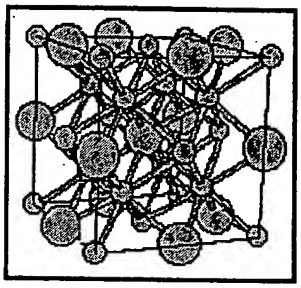
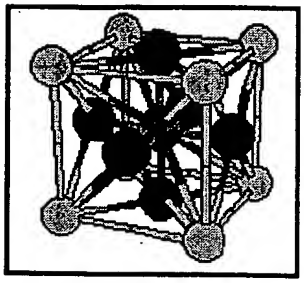


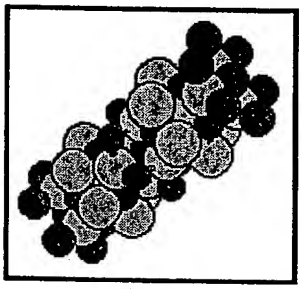
C Type



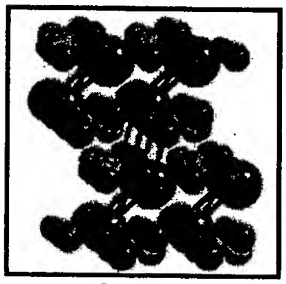
D Type



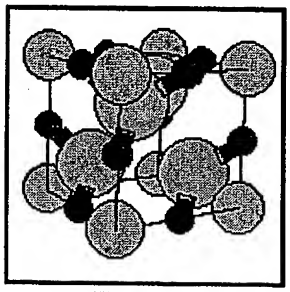
E Type



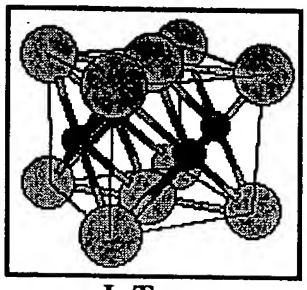
F Type



G Type



H Type



L Type

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Structures indexed by:

- Pearson Symbol
- Space Group
- Prototype

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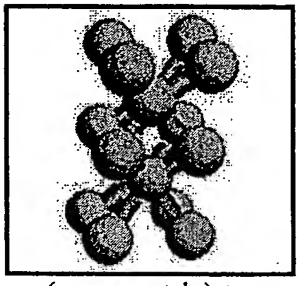
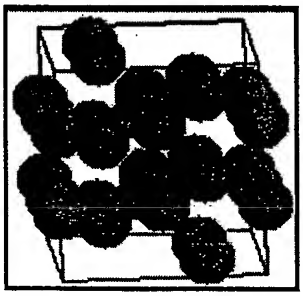
Index by Pearson Symbol

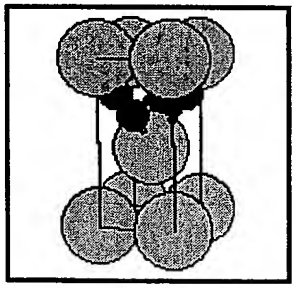
The Pearson symbol indicates the crystal symmetry and the number of atoms in the unit cell. For example, NaCl has a face-centered (F) cubic (c) structure with 8 atoms in the cube, so it is designated cF8. Cinnabar has 6 atoms in a hexagonal (h) primitive (P) cell, so it is designated hP6. Note that the Pearson symbol does not necessarily specify a unique structure (e.g., cF8).

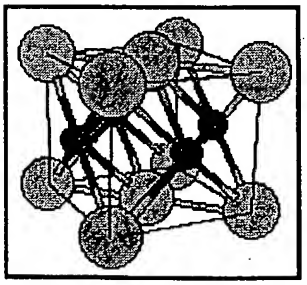
You will notice a striking similarity between the Pearson symbol categories and the space group categories.

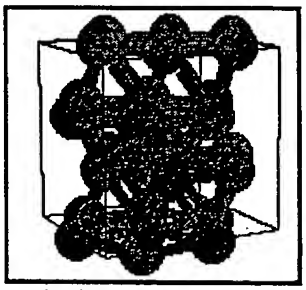
Pearson Symbol Categories:

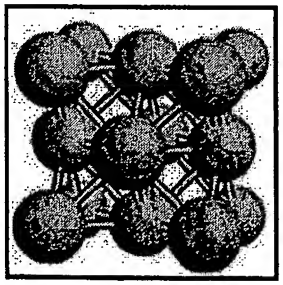

a (asymmetric) type


m (monoclinic) type


o (orthorhombic) type


t (tetragonal) type


h (hexagonal and rhombohedral) type


c (cubic) type

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Index by Space Group

Space groups are listed in the order they appear in the Crystallographic Tables.

Where it conflicts with the Crystallographic Tables we use the notation in *Pearson's Handbook*.

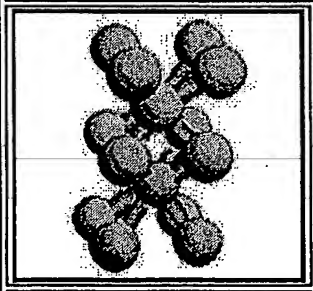
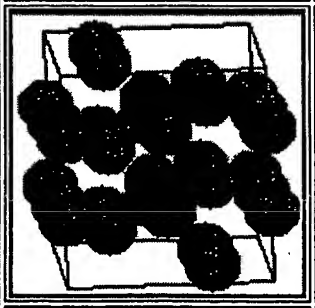
Space Group generators, Wyckoff positions, etc., are available online via the very useful Bilbao Crystallographic Server, and at the National Research Council of Canada's Generation of standard and alternate settings of the 230 Space Groups page. The easiest way to find information about a given space group is to use the Table of Space Group Symbols.

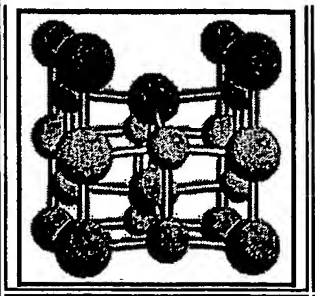
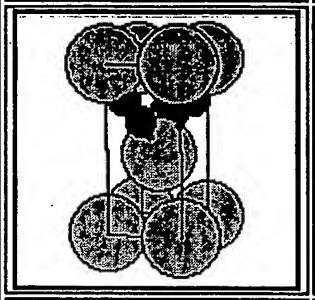
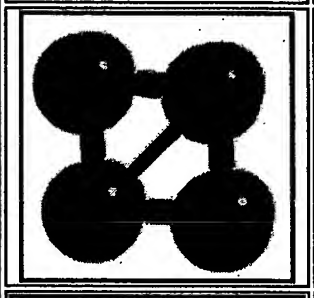
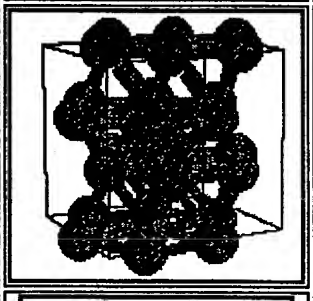
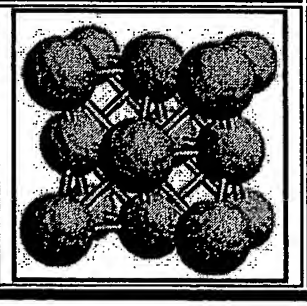
We also have more information on how space groups are presented here.

Each class of space groups corresponds to certain Pearson Symbols. Clicking on the appropriate symbol will take you to that part of the Pearson Symbol Index,

---

Space Group Classes:

Class		Pearson Symbols
	Triclinic Structures (#1-#2)	aPn
	Monoclinic Structures (#3-#15)	mPn mCn

	Orthorhombic Structures (#16-#74)	oPn oFn oIn oCn
	Tetragonal Structures (#75-#142)	tPn tIn
	Trigonal Structures (#143-#167)	hPn hRn
	Hexagonal Structures (#168-#194)	hPn
	Cubic Structures (#195-#230)	cPn cFn cIn

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Notes on individual crystallographers
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III. Nomenclature for crystal-chemical formulae

III.1. *General remarks*

An acceptable nomenclature for crystal-chemical formulae should exhibit the following general characteristics:

(1) It should be as simple and self-explanatory as possible.

(2) It should retain the chemical symbols of the elements and, whenever possible, follow the normal rules of chemical formulae.

(3) It should retain other widely used symbols (*e.g.* coordination number, dimensionality *etc.*) as far as possible.

(4) It should not introduce symbols which are already widely used but with a different meaning.

(5) It should be flexible, allowing symbols to be eliminated for simplification, or permitting the inclusion of extra symbols for additional information.

(6) It should be easy to print and suitable for computer use.

The proposed nomenclature for crystal-chemical formulae is based on the distribution of bond strengths. The spatial distribution of bond strengths in a structure can be either homogeneous or heterogeneous. If the distribution is *heterogeneous*, certain atoms are more tightly bonded together than others, resulting in finite groups or in assemblages that are infinite in one, two or three dimensions. These assemblages are considered as *structural units* and the remaining atoms as *interstitial atoms*.

If the spatial bond-strength distribution is *homogeneous*, two limiting situations may be discerned: either the structure is based on a three-dimensional framework (examples are diamond or cristobalite with directional bonds), or it is simply a packing of individual atoms (examples are helium, copper or sodium chloride with non-directional bonds). The corresponding sructural units are thus either a framework or the individual atoms, respectively.

There are five main categories of structural units, according to the kind of bond-strength distribution:

Dimensionality of structural unit	Category of structural unit

0-dimensional	individual atoms groups (*i.e.* rings, chain fragments, cages)
1-dimensional	chains
2-dimensional	sheets
3-dimensional	frameworks.

A structural unit may be considered to consist of subunits such as single atoms, polyhedra, single rings, single chains or single layers.

A structure can be considered to consist of structural units packed together, with interstitial atoms located between them. If the structural unit is a framework, the interstitial atoms or groups of atoms occupy holes within the framework.

Since the strengths of bonds cannot always be accurately quantified, some ambiguity may exist in assigning a structure to a given category.

III.2. *Fundamental features of notation*

III.2.1. *General crystal-chemical formulae*. Crystal-chemical formulae give detailed structural information on the *structural unit(s)*, their *constitution*, the *packing scheme*, the *interstitial atoms*, and the *coordination of the atoms* (both interstitial and those contained in the structural units).

Symbols for atoms belonging to the structural unit(s) are placed between square brackets, [ ], and the packing information between angle brackets, ⟨ ⟩. The information on constitution which relates to the structural unit as a whole is placed within curly brackets, { }. However, the constitutional information which relates to subunits of the structural unit(s) may be expressed either within curly brackets or as trailing superscripts to the chemical elements or subunits inside the structural unit.

Curly brackets with constitutional information precede and angle brackets for packing information immediately follow the structural unit to which they refer.

Information concerning interstitial atoms and/or groups of atoms should generally be placed before or after that on the structural unit(s) in the sequence that chemical formulae are usually written.

In accordance with IUPAC (1990) rules, the valency state of each atom is expressed immediately after its chemical symbol by a Roman numeral in parentheses [*e.g.* Fe(III)], a superscripted Roman numeral (*e.g.* Fe^{III}), or by a superscripted Arabic numeral followed by the sign + or - (*e.g.* Fe^{3+}).

The coordination of each atom, either interstitial or in the structural unit, is expressed within square brackets as a trailing superscript to the chemical symbol. If additional constitutional information related to subunits is given within the square brackets for the structural unit, then it should be placed between Japanese quotation marks (called `brackets') below), ⌈ ⌋, as an additional trailing superscript:

$A^{n+}{}^{[\,\lceil\,\rfloor\,]}$.

The general notation for a compound $A_aB_bC_cD_dE_eF_fG_g$ could thus be:

$$A_a^{[\alpha]}B_b^{[\beta]}\ \{\ \}\ [C_c^{[\gamma]}[\varphi]D_d^{[\delta]}[\chi]E_e^{[\varepsilon]}]\ \langle\ \rangle\ F_f^{[\xi]}G_g^{[\eta]}$$

interstitial atoms	constitution of structural unit	structural unit	packing of structural units	interstitial atoms.

Examples are given in § III.2.2 and Table 3.

Table 3: Examples of crystal-chemical formulae and *Ba*

Compound		Crystal-chemical formula	
He (hex.)	$^{0}_{\infty}[He]\langle h\rangle$	$[He]^{h}$	$^{3}_{\infty}$ |
Cu	$^{0}_{\infty}[Cu]\langle c\rangle$	$[Cu]^{c}$	$^{3}_{\infty}$ |
C (diamond)	$^{3}_{\infty}[C^{[4t]}]$	$^{3}_{\infty}[C]^{[4]}$	$^{3}_{\infty}$ |
NaCl	$Na^{[6]}{}^{0}_{\infty}[Cl^{[6]}]$	$Na^{o}[Cl]^{c}$	$^{3}_{\infty}$ |
SiO_2 (quartz)	$^{3}_{\infty}[Si^{[4t]}O_2]$	$^{3}_{\infty}[Si^{[4t]}[1;4]O_2]$	$^{3}_{\infty}$ |
SiO_2 (cristobalite)	$^{3}_{\infty}[Si^{[4t]}O_2]$	$^{3}_{\infty}[Si^{[4t]}[1;4]O_2]$	$^{3}_{\infty}$ |
FeS_2 (pyrite)	$Fe^{[6o]}\{^{0}_{\infty}\}[S_2^{[3;(1+2)]}]$	$Fe^{[6o]} \wedge [S_2^{[(3;1)t]}]$	Fe
FeS_2 (marcasite)	$Fe^{[6o]}\{^{0}_{\infty}\}[S_2^{[3;(1+2)]}]$	$Fe^{[6o]} \wedge [S_2^{[(3;1)t]}]$	Fe
$(Mg,Fe)_2SiO_4$ (olivine)	$(Mg,Fe)_2^{[6o]}\{^{0}_{\infty}\}[Si^{[4t]}O_4]$	$(Mg,Fe)_2^{[6o]}\{^{0}_{\infty}\}[Si^{[.4t]}O_4]$	(M
$MgAl_2O_4$ (spinel)	$^{3}_{\infty}[Mg^{[4t]}Al_2^{[6o]}O_4^{[1,3;12co]}]$	$Mg^{[.4t]}Al_2^{[.6o]}O_4$	M
$CaMgSi_2O_6$ (diopside)	$Ca^{[8]}Mg^{[6o]}\{^{1}_{\infty}\}[Si_2^{[4t]}[1;2]O_6]$		Ca

$KAl_3Si_3O_{10}(OH)_2$ (muscovite)	$K^{[6+6]}\{^{2}_{\infty}\}[Al_2^{[6o]}\{^{2}_{\infty}\}[(Al_{0.5}Si_{1.5})^{[4f]I[1;3]}O_5]_2(OH)_2]$	K
LaP_2 (HT form)	$La_4\{^{0}_{\infty}\}[P_2^{[;1]}P^{[;2]}]\{^{0}_{\infty}\}[P_2^{[;1]}P_3^{[;2]}]$	La
Ba_3AlSb_3	$Ba_6\{^{0}_{\infty}\}[Al_2^{[;4f]I[2;1]}Sb_6]$	
Ca_3AlAs_3	$Ca_3\{^{1}_{\infty}\}[Al^{[;4f]I[1;2]}As_3]$	
$(Mn,Fe)AlPO_4(OH)_2H_2O$ (eosphorite)	$(Mn,Fe)^{[6o]I[2;2]}Al^{[6o]I[1;2]}\{^{0}_{\infty}\}[P^{[4f]}O_4](OH)_2.H_2O$	
Na_3AlF_6 (cryolite)	$Na_3\{^{3}_{\infty}\}[Al^{[6o]I[1;6]}F_6]$	
$Ca_3Si_2O_7$ (rankinite)	$Ca_3\{^{0}_{\infty}\}[Si_2^{[4f]I[1;1]}O_7]$	
$Ca_3Si_2O_7$ (kilchoanite)	$Ca_6\{^{0}_{\infty}\}[Si^{[4f]I[0;0]}O_4]\{^{0}_{\infty}\}[Si_2^{[4f]I[1;1]}Si^{[4f][1;2]}O_{10}]$	

If several distinct structural units are present, each is considered separately with its information in curly brackets followed by that in square brackets, for example:

$$A_a^{[\alpha]}\{\,\}[B_b^{[\beta]}C_c^{[\gamma]}]\{\,\}[D_d^{[\delta]}E_e^{[\epsilon]}]\langle\,\rangle F_f^{[\zeta]}G_g^{[\eta]}.$$

The packing information within angle brackets describes the way the two different structural units pack together.

The hierarchy of bonds leads to a hierarchy of structural units when several degrees of bond strengths may be discerned in a structure. This often leads to weaker bond-strength units incorporating previous more strongly bonded units, and can be expressed by multiple brackets, with the central brackets referring to the structural unit having the strongest bonds:

$$A_a^{[\alpha]}\{\}[B_b^{[\beta]}\{\}[C_c^{[\gamma]}D_d^{[\delta]}E_e^{[\epsilon]}]\langle\,\rangle]\langle\,\rangle F_f^{[\zeta]}G_g^{[\eta]}.$$

The proposed formula can be used with any amount of any selection of structural information depending on the purpose of the study; see below.

III.2.2. *Constitution of structural units*. The constitution of a structural unit expresses its extensional and geometrical `structural'. *i.e.* the way the structural unit is built from its subunits, which may be polygons, polyhedra or any other clusters.

Some of the constitutional aspects are concerned with the structural unit as a whole, whereas other aspects are only concerned with the way each subunit is linked to other subunits. The former include *dimensionality, multiplicity, branchedness* and *periodicity*.

(i) The *dimensionality* is the number of dimensions in which a structural unit has infinite extension. It is zero for individual atoms and finite groups and one, two or three for infinite chains, sheets and frameworks, respectively. The corresponding symbols to be used in a crystal-chemical formula are $^{0}_{\infty}$, $^{1}_{\infty}$, $^{2}_{\infty}$ and $^{3}_{\infty}$.

The following specific symbols may be used instead of $^{0}_{\infty}$ for 0-dimensional structural units:

individual atom: {*a*}

group: {*g*}
- ring: {*r*} or ○
- chain fragment: {*f*} or ∧
- cage: {*k*} or Ⓥ

Examples are: $Cs^{2}\wedge[S_6]$, $Na^{4}Ⓥ[Si_4]$, $Cu_6\{r\}[Si_6O_{18}].6H_2O$.

If dimensionality is the only information expressed, the $^{n}_{\infty}$ and the pictorial symbols may be used without curly brackets. Otherwise, curly brackets are compulsory in order to avoid ambiguity.

The symbol {*a*} is not needed when several individual atoms, *A*, *B*, *C*, ..., considered as structural units, are written [*A*][*B*][*C*] ... . When only one atom symbol is placed within square brackets, it means that the structural unit is reduced to an individual atom. However, if the same atom symbols are written [*ABC*], then it is necessary to add {*a*} in front of the square brackets.

In the case of group structures, *e.g.* ring, chain fragment, and cage structures, the number of atoms of each chemical element within square brackets must be equal to the number of atoms of each chemical element in the finite group.

(ii) The *multiplicity* of a structural unit is the number of single subunits, *e.g.* polyhedra, single rings, single chains or single layers which are linked to form a complex structural unit of the same dimensionality.

(iii) With regard to *branchedness*, finite structural units and single chains are called unbranched if they contain no subunits that are linked to more than two other units. They are called branched if they do. In addition, complex structural units, which can be considered as formed by linking unbranched (branched) finite structural units or single chains, are described as unbranched (branched).

(iv) The *periodicity* of a structural unit of infinite extension is the number of subunits, excluding branches, within one repeat unit of the chain from which the structural unit can be generated by successive linking.

For details of concepts under (ii)-(iv) see Liebau (1982, 1985); a publication on their usage in the present formulae is in preparation.

The main constitutional aspects concerned only with *the way each subunit is linked to the other subunits* are *linkedness* and *connectedness*.

(i) The *linkedness* is the number L of peripheral atoms shared between two subunits. The value of linkedness is zero for an isolated subunit. It is one or two for two subunits sharing a corner or an edge, respectively, and it is three or more for two subunits sharing a face. The average linkedness value of a subunit may be non-integral if the given subunit shares corners plus edges with different adjacent subunits.

(ii) The *connectedness* of a subunit is the total number s of adjacent subunits with which it shares common atoms, irrespective of its linkedness with a particular adjacent subunit. A subunit may be singular (isolated), primary (linked to only one other subunit), secondary (linked to two others), *etc.*

The specific values L_1, L_2 *etc.* of linkedness and/or s of connectedness of a subunit are written within 'Japanese brackets' as trailing superscripts to its central atom, by analogy with the coordination symbols. The first entries in the Japanese brackets are the different values of L_n, separated from the value of s by a semicolon. The general formula for a structural unit with only one kind of subunit then reads

$$[A_m{}^{[L_1,L_2,\ldots;s]}B_n].$$

For example, SiO_2 exists in a number of polymorphs having different values of linkedness and connectedness of the SiO_4 tetrahedra:

fibrous silica:

$$^{1}_{\infty}[Si^{[4;2]}O_2];$$

quartz, cristobalite, coesite *etc.* :

$$^{3}_{\infty}[Si^{[4;4]}O_2];$$

and stishovite

$$^{3}_{\infty}[Si^{[6;1,1,1,1,1,1,1,1,2,2;10]}O_2],$$

abbreviated as $^{3}_{\infty}[Si^{[6;1,2;10]}O_2]$.

A structural unit can often be generated from a part of either lower or the same dimensionality by a simple geometrical process that usually represents an infinitely repeated translation. This imaginary geometrical process is called *condensation* because it emphasizes the way a chain can be generated from a group, a sheet from a chain, and a framework from a sheet. It also reveals certain similarities between different structural units, and a specific composite notation for the structural units has been developed

which emphasizes this interrelationship (§ V).

III.2.3. *Packing of structural units*. The *packing* of structural units expresses the three-dimensional arrangement in space. When the structural units are individual atoms, the known nomenclature for describing the packing of atoms (three-dimensional and layer-stacking descriptions) may be used. When the structural units are groups, their centres of gravity may be used with the same nomenclature as for the packing of atoms. However, this will be an incomplete description because of the lack of information on the orientation of the groups.

Packing of structural units in structures based on groups, infinite chains or sheets may be treated by layer description. Such a *layer description* consists of slicing the structure into layers which, by stacking, completely generate the original crystal structure. Structural units should be preserved intact in the process of slicing. The structure is then described by the packing of structural units in the layer and by a set of stacking operators.

The layer description can also be applied to framework structures taking into consideration the fact that the units operated upon are parts of a single framework.

With respect to the nomenclature for the packing of structural units, only the symbols for cubic closest packing, *c*, and hexagonal closest packing, *h*, and their sequential combination are adopted here. When no other packing information is provided these symbols may be given as trailing superscripts to the square brackets which contain the structural unit. In this case, angle brackets are not compulsory. Any other packing information, particularly the packing (or stacking) symbolism used by individual authors should be given in angle brackets *on the line*.

$$[ABC]^{c} \text{ or } [ABC]\langle\ldots\rangle.$$

If packing information is to be given for a set of atoms which does not constitute a structural unit, the symbol should be placed within vertical bars followed by the packing information:

$$|ABC|^{c} \text{ or } |ABC|\langle\ldots\rangle.$$

Next Up Previous

Next: IV. The Bauverband approach **Up:** Nomenclature of Inorganic Structure Types **Previous:** II. Coordination of the atoms

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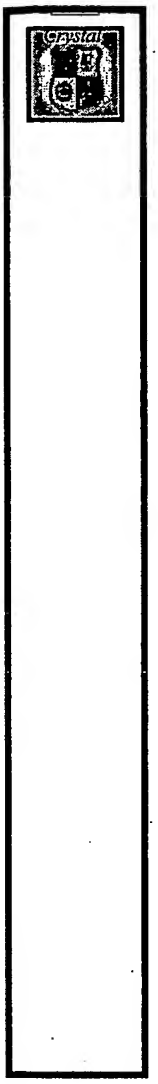

Crystal Lattice Structures:

Reference Date: 1 Jul 2001
Last Modified: 22 Feb 2006

Prototype Index

- This is an index of the various crystal structures by prototype compound. Note that these are in the logical alphabetical order. Thus what is usually called Cu_3Au is listed as $AuCu_3$, and rock salt as ClNa.
- Hypothetical compounds such as BCT5 are listed with their proposed constituents (here, Si). If an element or compound is associated with more than one prototype the most common prototype is listed first.

Prototype	Pearson's Symbol	*Strukturbericht* Designation	Space Group	Notes
AgAsMg	cF12	$C1_b$	F$\bar{4}$3m (#216)	half-Heusler
$AgAuTe_4$	mP12	$E1_b$	P2/c (#13)	
AgC_2KN_2	hP36	$F5_{10}$	P$\bar{3}$1c (#163)	Usually written $KAg(CN)_2$
Ag_2O	cP6	C3	Pn$\bar{3}$m (#224)	Cuprite
AgZn (η)	hP9	B_b	P$\bar{3}$ (#147)	
AlB_2	hP3	C32	P6/mmm (#191)	hexagonal omega
AlB_4Mg	hP6		P6/mmm (#191)	doubled omega
Al_4Ba	tI10	$D1_3$	I4/mmm (#139)	
$AlCCr_2$	hP8		$P6_3$/mmc (#194)	some MAX phase
Al_5C_3N	hP18	$E9_4$	$P6_3$mc (#186)	
Al_2CdS_4	tI14	E3	I$\bar{4}$ (#82)	
$AlCl_3$	mC16	$D0_{15}$	C2/m (#12)	
Al_2Cu	tI12	C16	I4/mcm (#140)	
$AlCu_2Mn$	cF16	$L2_1$	Fm$\bar{3}$m (#225)	Heusler

AlF_3	hR8	$D0_{14}$	R32 (#155)	
$AlFe_3$	cF16	$D0_3$	$Fm\bar{3}m$ (#225)	
Al_2MgO_4	cF56	$H1_1$	$Fd\bar{3}m$ (#227)	Spinel
AlN_3Ti_4	hP16		$P6_3/mmc$ (#194)	MAX phase
Al_3Ni_2	hP5	$D5_{19}$	$P\bar{3}m1$ (#164)	
Al_2O_3 (α)	hR10	$D5_1$	$R\bar{3}c$ (#167)	Corundum
$AlPS_4$	oP12		P222 (#16)	
AlPd	hR26		$R\bar{3}$ (#148)	
AlSb	cP16		$Pa\bar{3}$ (#205)	SC16
Al_3Ti	tI8	$D0_{22}$	I4/mmm (#139)	
$Al_{12}W$	cI26		$Im\bar{3}$ (#204)	
Al_3Zr	tI16	$D0_{23}$	I4/mmm (#139)	
As (α)	hR2	A7	$R\bar{3}m$ (#166)	
As_3Co	cI32	$D0_2$	$Im\bar{3}$ (#204)	Skutterudite
$AsCu_3S_4$	oP16	$H2_5$	$P2m_1$ (#31)	Enargite
$AsCu_3S_4$	cP8		$P\bar{4}3m$ (#215)	Lazarevicite
AsGa	oI4		Imm2 (#44)	> 24 GPa
AsK_3S_4	oP32		$Pna2_1$ (#33)	
$AsKSe_2$	aP16		P1 (#1)	
$AsNa_3$	hP8	$D0_{18}$	$P6_3/mmc$ (#194)	
AsNi	hP4	$B8_1$	$P6_3/mmc$ (#194)	
AsTi	hP8	B_i	$P6_3/mmc$ (#194)	
AuCd	oP4	B19	Pmma (#51)	
AuCu	tP2	$L1_0$	P4/mmm (#123)	
$AuCu_3$	cP4	$L1_2$	$Pm\bar{3}m$ (#221)	
$AuTe_2$	mC6	C34	C2/m (#12)	Calaverite
$AuTe_2$	oP24	C46	Pma2 (#28)	Krennerite

B (α)	hR12		R$\bar{3}$m (#166)	
B (β)	hR105		R$\bar{3}$m (#166)	
B	tP50	A_g	$P4_2/nnm$ (#134)	
B_2C_2Mg	oC80		Cmca (#64)	
B_6Ca	cP7	$D2_1$	Pm$\bar{3}$m (#221)	
BCr	oC8	B33	Cmcm (#63)	
BFe	oP8	B27	Pnma (#62)	
B_4Mg	oP20		Pnma (#62)	
BMo	tI16	B_g	$I4_1/amd$ (#141)	
B_5Mo_2	hR7	$D8_i$	R$\bar{3}$m (#166)	
BN	hP4	B_k	$P6_3/mmc$ (#194)	
BN	hP4	B12	$P6_3mc$ (#186)	
BO_4P	tI12	$H0_7$	I$\bar{4}$ (#82)	
B_2Pd_5	mC28		B2/b (#15)	
$B_{12}U$	cF52	$D2_f$	Fm$\bar{3}$m (#225)	
B_5W_2	hP14	$D8_h$	$P6_3/mmc$ (#194)	
$Ba_2Cu_3O_{7-x}Y$	oP14		Pmmm (#47)	
$BaHg_{11}$	c36	$D2_e$	Pm$\bar{3}$m (#221)	
$(Ba,La)_2CuO_4$	tI14		I4/mmm (#139)	
BaPtSb	hP3		P$\bar{6}$m2 (#187)	
BiI_3	hR8	$D0_5$	R$\bar{3}$ (#148)	
Bi_2Te_3	hR5	C33	R$\bar{3}$m (#166)	
C	cF8	A4	Fd$\bar{3}$m (#227)	Diamond
C	hP4	A9	$P6_3/mmc$ (#194)	Graphite
C	hP4		$P6_3mc$ (#186)	Buckled Graphite

C	hR2		R$\bar{3}$m (#166)	Rhombohedral Graphite
C	hP4		$P6_3/mmc$ (#194)	Lonsdaleite
C (3-ring)	hP6		$P6_3/mmc$ (#194)	3-member ring
C (4-ring)	tI8		I4/mmm (#139)	4-member ring
$CCaO_3$	hR10		R$\bar{3}$c (#167)	Calcite
C_2CeNi	oC8		Amm2 (#38)	
CClN	oP6		Pmmn (#59)	Cyanogen Chloride
C_3Cr_7	oP40	$D10_1$	Pnma (#62)	
CFe_2	oP6		Pnnm (#58)	
CFe_3	oP16	$D0_{11}$	Pnma (#62)	Cementite
CFe_3	hP8		$P6_322$ (#182)	Bainite
CFe_4	cP5		P$\bar{4}$3m (#215)	
CFe_3W_3	cF112	$E9_3$	Fd$\bar{3}$m (#227)	
C_8H_8	hR16		R$\bar{3}$ (#148)	Solid Cubane
CKNS	oP16	$F5_9$	Pbcm (#57)	
CMo	hP12		$P6_3/mmc$ (#194)	some MAX phase
CO	cP8	B21	$P2_13$ (#198)	
C_3Pu_2	cI40	$D5_c$	I$\bar{4}$3d (#220)	
CSi	hP12		$P6_3mc$ (#186)	Moissanite-6H
CSi	hP8		$P6_3mc$ (#186)	Moissanite-4H
CSi	hR18		R3m (#160)	Moissanite-9R
CW	hP2	B_h	P$\bar{6}$m2 (#187)	
$CaCl_2$	oP6	C35	Pnnm (#58)	
$CaCu_5$	hP6	$D2_d$	P6/mmm (#191)	
CaF_2	cF12	C1	Fm$\bar{3}$m (#225)	Fluorite
	mC40		C2/c (#15)	Esseneite

$CaFeO_6Si_2$				
Ca_7Ge	cF32		Fm3m (#225)	
$Ca_{33}Ge$	cF48		Fd3m (#227)	also CTi_2
$CaIn_2$	hP6		$P6_3/mmc$ (#194)	
CaO_3Ti	cP5	$E2_1$	Pm3m (#221)	Cubic Perovskite
CaO_3Ti	oP20		Pnma (#62)	Perovskite
CdSb	oP16	B_e	Pbca (#61)	
CdTe	oP2		Pmm2 (#25)	
Cf	aP4		P(-1) (#2)	
ClCs	cP2	B2	Pm3m (#221)	
ClNa	cF8	B1	Fm3m (#225)	Rock Salt
Co_2Si	oP12	C37	Pnma (#62)	
CoSn	hP6	B35	P6/mmm (#191)	
CoU	cI16	B_a	$I2_13$ (#199)	
$CrCl_3$	hP24	$D0_4$	$P3_112$ (#151)	
CrFe (σ)	tP30	$D8_b$	$P4_2/mnm$ (#136)	
$CrFe_4Ni_3$	cI16		Im3m (#229)	Hypothetical Ferrite Structure
$CrFe_8MoNi_6$	cP16		Pm3m (#221)	Hypothetical Ferrite Structure
$CrFe_{12}Ni_3$	cI32		Im3m (#229)	Hypothetical Austenite Structure
$CrFe_{18}Ni_8$	cF108		Fm3m (#225)	Hypothetical Austenite Structure
$CrFe_{20}Ni_6$	cI54		Im3m (#229)	Hypothetical Ferrite Structure
$CrFe_{25}Ni_6$	cP32		Pm3m (#221)	Hypothetical Austenite Structure
$Cr_9Fe_{16}Ni_7$	cF128		Fm3m (#225)	Hypothetical Ferrite Structure
$CrNaS_2$	hR4	$F5_1$	R3m (#166)	Caswellsilverite

Cr_3Si	cP8	A15	$Pm\bar{3}n$ (#223)	
$CrSi_2$	hP9	C40	$P6_222$ (#180)	
CrTi	hP3	C6	$P\bar{3}m1$ (#164)	omega phase
Cu	cF4	A1	$Fm\bar{3}m$ (#225)	fcc
$CuFeS_2$	tI16	$E1_1$	$I\bar{4}2d$ (#122)	Chalcopyrite
Cu_2FeS_4Sn	tI16	$H2_6$	$I\bar{4}2m$ (#121)	Stannite
Cu_2Mg	cF24	C15	$Fd\bar{3}m$ (#227)	Cubic Laves
Cu_4MgSn	cF24	$C15_b$	$F\bar{4}3m$ (#216)	
CuO	mC8	B26	C2/c (#15)	Tenorite
CuPt	hR32	$L1_1$	$R\bar{3}m$ (#166)	
CuS	hP12	B18	$P6_3/mmc$ (#194)	
Cu_3S_4V	cP8	$H2_4$	$P\bar{4}3m$ (#215)	Sulvanite
Cu_2Sb	tP6	C38	I4/nmm (#129)	
$CuSbS_2$	oP16	$F5_6$	Pnma (#62)	
CuTe	oP4		Pmmn (#59)	
Cu_2Te	hP6	C_h	P6/mmm (#191)	
CuTi (γ)	tP4	B11	P4/nmm (#129)	
$CuTi_3$	tP4	$L6_0$	P4/mmm (#123)	
Cu_3Ti (β)	oP8	$D0_a$	Pmmn (#59)	
F_4Si	cI10		$I\bar{4}3m$ (#217)	
FTl	oF8	B24	Fmmm (#69)	
FeO_3Ti	hR10		$R\bar{3}$ (#148)	Ilmenite
Fe_2P	hP9	C22	P321 (#150)	Original Structure
Fe_2P	hP9	C22	$P\bar{6}2m$ (#189)	Revised Structure
FeS_2	cP12	C2	$Pa\bar{3}$ (#205)	Pyrite
FeS_2	oP6	C18	Pnnm (#58)	Marcasite
FeS_2	aP12		P1 (#1)	

FeSi	cP8	B20	$P2_13$ (#198)	
Ga (α)	oC8	A11	Cmca (#64)	
Ga_2Hf	tI24		$I4_1/amd$ (#141)	
Ga_4Ni	cI40		I23 (#197)	
Ga_4Ni_3	cI112		$Ia\bar{3}d$ (#230)	
Ga_3Pt_5	oC16		Cmmm (#65)	
GeS	oP8	B16	Pnma (#62)	
GeS_2	oF72	C44	Fdd2 (#43)	
H_3N	cP16	D1	$P2_13$ (#198)	Ammonia
H_2Th	tI6	L'2	I4/mmm (#139)	
Hg (α)	hR1	A10	$R\bar{3}m$ (#166)	Rhombohedral
$HgBr_2$	oC12	C24	$Cmc2_1$ (#36)	
$HgCl_2$	oP12	C25	Pnma (#62)	
HgS	hP6	B9	$P3_221$ (#154)	Cinnabar
$HgSn_{6-10}$ (γ)	hP1	A_f	P6/mmm (#191)	Simple Hexagonal
I_2	oC8	A14	Cmca (#64)	
I_2P_4	aP6		$P\bar{1}$ (#2)	
In	tI2	A6	I4/mmm (#139)	fct
$InNi_2$	hP6	$B8_2$	$P6_3/mmm$ (#194)	
Ir_3Si	tI16	$D0'_c$	I4/mcm (#140)	
$KClO_3$	mP10	$G0_6$	$P2_1/m$ (#11)	
La (α)	hP4	A3'	$P6_3/mmc$ (#194)	
La_2O_3	cI5		$Im\bar{3}m$ (#229)	
Li	cI16		$I\bar{4}3d$ (#220)	High-Pressure cI16 phase
Li_3N	hP4		P6/mmm (#191)	

$LiNbO_3$	hR10		R3c (#161)	Ferroelectric phase
$LiNbO_3$	hR10		$R\bar{3}c$ (#167)	Paraelectric phase
Mg	hP2	A3	$P6_3/mmc$ (#194)	hcp
$MgNi_2$	hP24	C36	$P6_3/mmc$ (#194)	Hexagonal Laves
Mg_2Ni	hP18		$P6_222$ (#180)	
$MgZn_2$	hP12	C14	$P6_3/mmc$ (#194)	Hexagonal Laves
Mn (α)	cI58	A12	I43m (#217)	
Mn (β)	cP20	A13	$P4_132$ (#213)	
MnP	oP8	B31	Pnma (#62)	
$Mn_{12}Th$	tI26	$D2_b$	I4/mmm (#139)	
$MoNi_4$	tI10	$D1_a$	I4/m (#87)	
$MoPt_2$	oI6		Immm (#71)	
MoS_2	hP6	C7	$P6_3/mmc$ (#194)	
$MoSi_2$	tI6	$C11_b$	I4/mmm (#139)	
N (α)	cP8		$Pa\bar{3}$ (#205)	αN_2
N (γ)	tP4		$P4_2/mnm$ (#136)	γN_2
NaTl	cF16	B32	$Fd\bar{3}m$ (#227)	
NbO	cP6		Pm3m (#221)	
NbP	tI8		$I4_1/amd$ (#141)	``40"
NiS	hR6	B13	R3m (#160)	
NiSSb	cP12	$F0_1$	$P2_13$ (#198)	Ullmanite
Ni_3S_2	hR5	$D5_e$	R32 (#155)	
Ni_3Sn	hP8	$D0_{19}$	$P6_3/mmc$ (#194)	
NiTi	mP4		$P2_1/m$ (#11)	
	cF96		$Fd\bar{3}m$ (#227)	

$NiTi_2$				
Np (α)	oP8	A_c	Pnma (#62)	
Np (β)	tP4	A_d	P4/nmm (#129)	
O_2 (α)	mC4		C2/m (#12)	
O_2 (β)	hR2		R$\bar{3}$m (#166)	
OPb	tP4	B10	P4/nmm (#129)	
$O_3PbTi_{1-x}Zr_x$	tP5		P4mm (#99)	Tetragonal PZT ($x > 0.52$)
$O_3PbTi_{0.48}Zr_{0.52}$	mC10		Cm (#8)	Monoclinic PZT
O_4Pt_3	cI14		Im$\bar{3}$m (#229)	
O_3Re (α)	cP4	$D0_9$	Pm$\bar{3}$m (#221)	
O_3Sb_2	oP20	$D5_{11}$	Pccn (#56)	
O_2Si (β)	hP9	C8	$P6_222$ (#180)	high Quartz
O_2Si (α)	hP9		$P3_221$ (#154)	low Quartz
O_2Si	hP12	C10	$P6_3/mmc$ (#194)	β Tridymite
O_2Si	cF24	C9	Fd$\bar{3}$m (#227)	Ideal β-Cristobalite
O_2Si	tP12		$P4_12_12$ (#92)	α Cristobalite
O_2Si	tP36		$P4_12_12$ (#92)	Keatite
O_4SiZr	tI24		$I4_1/amd$ (#141)	Zircon
O_2Ti	tP6	C4	$P4_2/mnm$ (#136)	Rutile
O_2Ti	tI12	C5	$I4_1/amd$ (#141)	Anatase
O_2Ti	oP24	C21	Pbca (#61)	Brookite
O_2Zr	mP12	C43	$P2_1/c$ (#14)	Baddeleyite
P	oC8	A17	Cmca (#64)	black Phosphorus
P	mP84		P2/c (#13)	monoclinic

				Phosphorus
$PPrS_4$	tI96		$I4_1/acd$ (#142)	
Pa (α)	tI2	A_a	I4/mmm (#139)	bct
$PbCl_2$	oP12	C23	Pnma (#62)	bct
PdS	tP16	B34	$P4_2/m$ (#84)	
$PdSn_2$	oC24	C_e	Aba2 (#41)	
Po (α)	cP1	A_h	Pm3m (#221)	Simple Cubic
Po (β)	hR1	A_i	R3̄m (#166)	
PtS	tP4	B17	$P4_2/mmc$ (#131)	
$PtSn_4$	oC20	$D1_c$	Aba2 (#41)	$PdSn_4$
Pu (α)	mP16		$P2_1/m$ (#11)	
Pu (β)	mC34		B2/m (#12)	Alternate Orientation
Pu (γ)	oF8		Fddd (#70)	
$ReSi_2$	oI6		Immm (#71)	
S (α)	oF128	A16	Fddd (#70)	
S_3Sb_2	oP20	$D5_8$	Pnma (#62)	
S_2Si	oI12	C42	Ibam (#72)	
SSn	oP8	B29	Pnma (#62)	
SZn	cF8	B3	F43m (#216)	Zincblende
SZn	hP4	B4	$P6_3mc$ (#186)	Wurtzite
Sb_2Tl_7	cI54		Im3̄m (#229)	
Se (α)	mP64	A_k	$P2_1/c$ (#14)	
Se (β)	mP32	A_l	$P2_1/c$ (#14)	
Se (γ)	hP3	A8	$P3_121$ (#152)	
SeTl	tI16	B37	I4/mcm (#140)	$AlKTe_2$
Si	cI16		Ia3̄ (#206)	BC8
Si	tP12		$P4_32_12$ (#96)	ST12

Si_{34}	cF136		$Fd\bar{3}m$ (#227)	Clathrate
Si_{46}	cP46		$Pm\bar{3}n$ (#223)	Clathrate
Si	tI4		I4/mmm (#139)	BCT5
Si_2Ti	oF24	C54	Fddd (#70)	
SiU_3	tI16	$D0_c$	I4/mcm (#140)	
Si_2U_3	tP10	$D5_a$	P4/mbm (#127)	
Si_2Zr	oC12	C49	Cmcm (#63)	
Sm (α)	hR3	C19	$R\bar{3}m$ (#166)	
Sn	tI4	A5	$I4_1/amd$ (#141)	White (β) Tin
Te	mP4		$P2_1$ (#4)	high-pressure Te
U (α)	oC4	A20	Cmcm (#63)	
U (β)	tP30	A_b	$P4_2/mnm$ (#136)	
W	cI2	A2	$Im\bar{3}m$ (#229)	bcc

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Structures indexed by:

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